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Multi-fluid Model of Exothermic Fields in Explosions

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1. Formulation

Proposed here is a multi-fluid extension of our multi-component model [1] of unmixed combustion in explosions. We recognize three fluids: *Fuel-F* and *Air-A* forming combustion *Products-P* at thermodynamic equilibrium. We consider the inviscid exothermic-flow limit [2]—where all molecular transport phenomena can be disregarded; thus, the Reynolds number $Re \to \infty$; the Peclet number for both heat and mass diffusion $Pe \to \infty$; the Damköhler number $Da \to \infty$, and the Mach number $Ma > 0$. As is typical of combustion in unmixed systems [3], fuel and air react in stoichiometric proportions σ called *Reactants-R.*

2. Conservation Equations

In the limit of $Re \to \infty$, the *mixture—m* is governed by the *Gasdynamic Conservation Laws:*

Mass: $$\partial_t \rho_m + \nabla \cdot (\rho_m \mathbf{u}) = 0 \qquad (1)$$

Momentum: $$\partial_t \rho_m \mathbf{u} + \nabla \cdot (\rho_m \mathbf{u}\mathbf{u}) = -\nabla p_m \qquad (2)$$

Energy: $$\partial_t \rho_m E_m + \nabla \cdot (\rho_m E_m \mathbf{u}) = [u_P - u_R](1+\sigma)\dot{\rho}_e \qquad (3)$$

where ρ, u, p and $\mathbf{u}$ denote density, internal energy, pressure and velocity vector, respectively, while $E_m \equiv u_m + \mathbf{u}\cdot\mathbf{u}/2$ and $[u_P - u_R]$ represents the energy transformation from R to P. To evaluate the pressure in fluid K, one needs to know its density and energy (i.e., $p_K = p_K(\rho_K, u_K)$ where K=F,A,P); these are obtained from *Mass-Energy Conservation Laws* for each fluid; at $Pe \to \infty$ they acquire the form

F: $$\partial_t \rho_F + \nabla \cdot (\rho_F \mathbf{u}) = -\dot{\rho}_e \quad \& \quad \partial_t \rho_F u_F + \nabla \cdot (\rho_F u_F \mathbf{u}) = -p_F \nabla \cdot \mathbf{u} - u_F \dot{\rho}_e \qquad (4a,b)$$

A: $$\partial_t \rho_A + \nabla \cdot (\rho_A \mathbf{u}) = -\sigma\dot{\rho}_e \quad \& \quad \partial_t \rho_A u_A + \nabla \cdot (\rho_A u_A \mathbf{u}) = -p_A \nabla \cdot \mathbf{u} - u_A \sigma \dot{\rho}_e \qquad (5a,b)$$

P: $$\partial_t \rho_P + \nabla \cdot (\rho_P \mathbf{u}) = (1+\sigma)\dot{\rho}_e \quad \& \quad \partial_t \rho_P u_P + \nabla \cdot (\rho_P u_P \mathbf{u}) = -p_P \nabla \cdot \mathbf{u} + u_P (1+\sigma) \dot{\rho}_e \qquad (6a,b)$$

m: $$\rho_m \equiv \rho_F + \rho_A + \rho_P \quad \& \quad u_m \equiv (\rho_F u_F + \rho_A u_A + \rho_P u_P)/\rho_m \qquad (7)$$

Combustion influences these fields only at the *exothermic front-e,* which is a sink ($\dot{\rho}_e$) for F & A and a source for P. The equations are integrated by a higher order Godunov method.

Adaptive Mesh Refinement provides enough mesh resolution to capture the mixing structures on the grid—so no turbulence model is needed [1].

3. Exothermic Front

According to the approximation $Da \to \infty$, the front [1] is represented as a Dirac delta function, δ, located at the stoichiometric contour , $\mathbf{x}_e(t_e)$:

$$\dot{\rho}_e \equiv \begin{cases} \rho_F \delta(\mathbf{x}-\mathbf{x}_e, t-t_e) & (1 \le \lambda_e < \infty) \\ 0 & (\lambda = 0, \infty) \\ \rho_A \delta(\mathbf{x}-\mathbf{x}_e, t-t_e)/\sigma & (0 < \lambda_e < 1) \end{cases} \tag{8}$$

where $\lambda(\mathbf{x}, t) \equiv (A - F\ ratio)/\sigma$, which varies throughout the flow field due to mixing.

4. Thermodynamics

Thermodynamic properties of the fluids are displayed in the Le Chatelier diagram (Fig. 1) of

$$\mathrm{W}_K \equiv (pv)_K / \mathrm{w}_{Ai} \qquad \& \qquad \mathrm{U}_K \equiv (\mathrm{u}_K - \mathrm{u}_{0K})/\mathrm{C}_A \mathrm{w}_{Ai} = \mathrm{Q}_K + \mathrm{k}_K \mathrm{W}_K \tag{9}$$

In an exothermic cell, *F* and *A* combine in stoichiometric proportions forming a point on *curve-R*; combustion transforms that point to one on *curve-P*. If the system is adiabatic, this transformation occurs initially at constant pressure and enthalpy (point *hp*), and at the final stage of combustion it occurs at constant energy and volume (point *uv*).

5. Illustration

This *Model* was used to simulate the combustion of the expanded detonation products from a 1-kg charge of TNT with air in a $V =$ 16.6-m^3 chamber. Figure 2 shows the measured enhancement of pressure due to combustion [4]. The mean (volume-averaged) fluid densities and energies from the simulation are presented in Figs. 3 and 4. The mass fraction of fuel consumed is shown in Fig. 5. The calculated pressure history agrees with data (Fig. 6).

6. Conclusion

Combustion in the *Multi-Fluid Model* is treated material transformations in the Le Chatelier plane (rather than "heat release" found in traditional models). This is the only way to construct a thermodynamically-consistent representation of the fluids. The *exothermic front* provides an extraordinarily sharp representation of turbulent combustion fields—which are normally clouded by a myriad of diffusional effects.

References

[1] Kuhl, A. L., Ferguson, R. E., and Oppenheim, A. K., "Gasdynamic Model of Turbulent Exothermic Fields in Explosions", *Advances in Combustion Science—in Honor of Ya. B. Zel'dovich, Progress in Astronautics and Aeronautics Series*, **173**, AIAA, Washington, DC (1997), pp. 251-261.

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[3] Zel'dovich, Ya. B., "K Teorii Goreniya Ne Peremeshannykh Gazov" ("On the Theory of Combustion of Initially Unmixed Gases") *Zh. Tekh. Fiz.*, **19** (10), 1949, pp. 1199-1210.

[4] Kuhl, A. L., Ferguson, R. E. and Oppenheim, A. K., "Gasdynamics of Combustion of TNT Products in Air", *Archivum Combustionis* (in press).

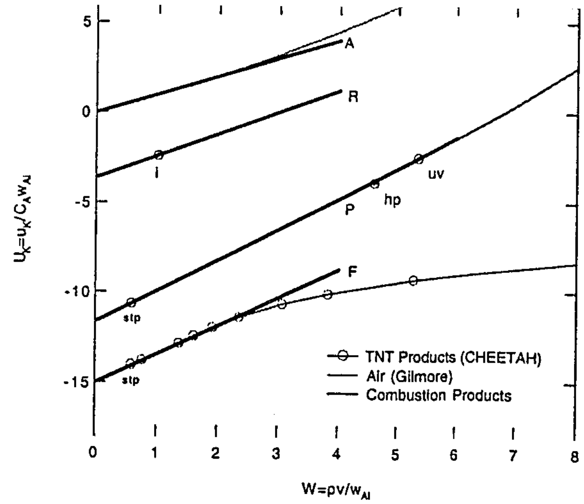

Fig. 1. Le Chatelier diagram for combustion of TNT detonation products in air.

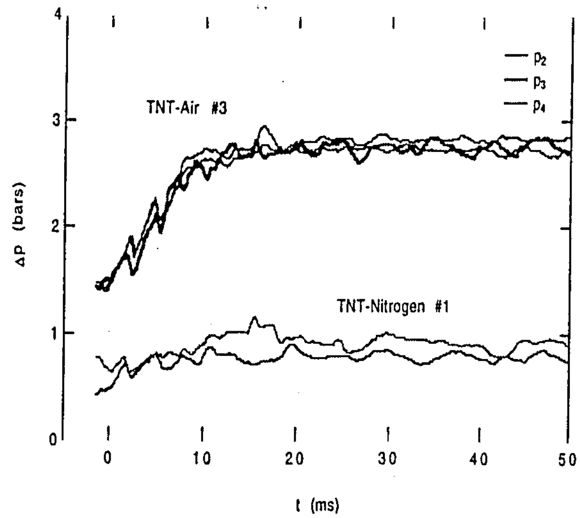

Fig. 2. Mean pressure histories for a 1-kg TNT explosion in air and N_2 ($V=17m^3$).

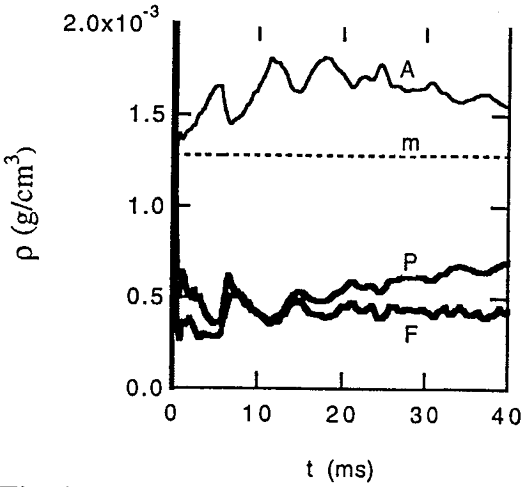

Fig. 3. Mean density histories of the fluids.

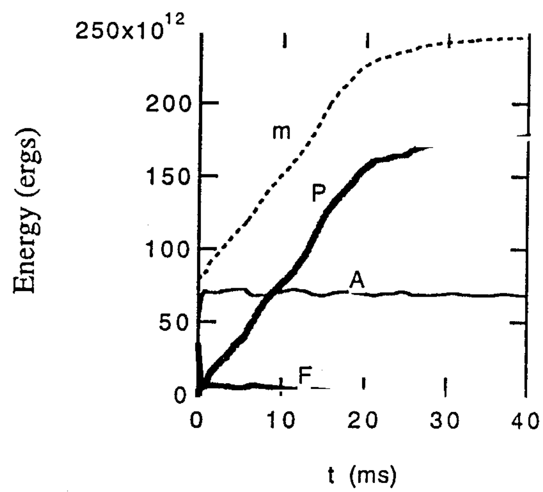

Fig. 4. Mean energy histories of the fluids.

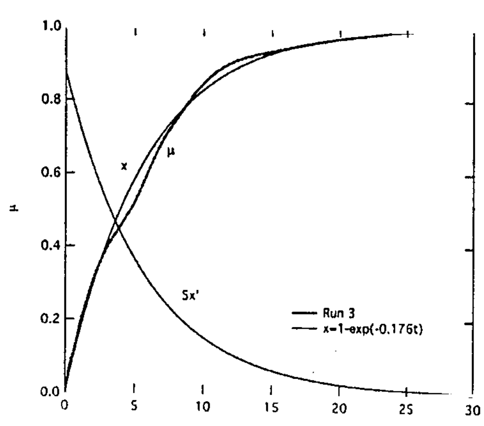

Fig. 5. Mass-fraction of fuel consumed.

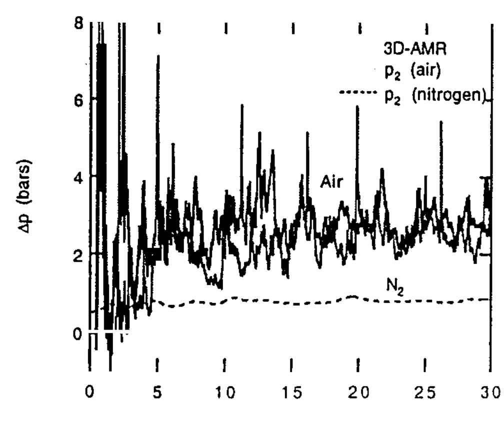

Fig. 6. Pressure history comparison.

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ABSTRACT

A *Multi-fluid Model* is proposed for turbulent combustion in explosions at infinitely-large Reynolds, Peclet & Damköhler numbers. It is based on the ***gasdynamic conservation laws*** for the mixture, augmented ***mass-energy conservation laws*** for each fluid (fuel-*F*, oxidizer-*A* and products-*P*). Combustion is treated as material transformations in the Le Chatelier plane—rather than "heat release" found in traditional models. This allows one to construct thermodynamically-consistent representations of the fluids. Such transformations occur at an ***exothermic front***—which represents, simultaneously, a ***sink*** for *F & A* and ***source*** of *P*. The front is represented by a Dirac delta function at the stoichiometric contour in the turbulent field. This *Model* then provides an extraordinarily clear picture of turbulent combustion fields, which are normally clouded by a myriad of diffusional effects.

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